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Remarks on the Modified Second Zagreb Index on a Line Graph

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Dedicated to the memory of Professor Ćemal Dolićanin (1945–2023)

Abstract: Let $G=(V,E)$, $V=\{v_1,v_2,\dots,v_n\}$, be a simple graph of order n and size m. Denote by $\Delta=d_1\geq d_2\geq\cdots\geq d_n=\delta$, $d_i=d(v_i)$, and $\Delta_e=d(e_1)\geq d(e_2)\geq\cdots\geq d(e_m)=\delta_e$, sequences of vertex and edge degrees, respectively. If vertices v_i and v_j are adjacent in G, we write $i\sim j$. The modified second Zagreb index is defined as $M_2^*(G)=\sum_{i\sim j}\frac{1}{d_id_j}$. In this paper we determine some new upper and lower bounds on $M_2^*(G)$ for a line graph $L(G)$ of G.
Keywords: graphs, topological indices, degree-based invariants.

1 Introduction

Let $G=(V,E)$, $V=\{v_1,v_2,\dots,v_n\}$, be a simple graph with n vertices, m edges with vertex–degree sequence $\Delta=d_1\geq d_2\geq\cdots\geq d_n=\delta>0$, $d_i=d(v_i)$, and edge degree sequence $\Delta_e=d(e_1)\geq d(e_2)\geq\cdots\geq d(e_m)=\delta_e$. If vertices v_i and v_j are adjacent in G, we write $i\sim j$. Likewise, if edges e_i and e_j are adjacent in G, we write $e_i\sim e_j$.

In graph theory, a graph invariant is property of the graph that is preserved by isomorphisms. The graph invariants that assume only numerical values are usually referred to as topological indices in chemical graph theory. Hundreds of various topological indices have been introduced in mathematical chemistry literature in order to describe physical and chemical properties of molecules. Various mathematical properties of topological indices have been investigated, as well. As topological indices have been defined for quantifying information of graphs, this area could be classified into the so called quantitative graph theory (see, for example [6, 13–15]).

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Many of topological indices are defined as simple functions of the degree sequence of (molecular) graph. In what follows we recall definitions of indices that are of interest for the present work.

The first Zagreb index, $M_1(G)$, is defined as the sum of the squares of the degrees of the vertices [8]

$$M_1(G) = \sum_{i=1}^{n} d_i^2 = \sum_{i\sim j} (d_i + d_j),$$

and the second Zagreb index as the sum of the product of the degrees of adjacent vertices [7]

$$M_2(G) = \sum_{i\sim j} d_i d_j .$$

The modified second Zagreb index $M_2^*(G)$ is a vertex-degree-based graph invariant introduced in [11]. It is defined by

$$M_2^*(G) = \sum_{i\sim j} \frac{1}{d_i d_j} .$$

Note that this topological index is also ment under the names variable second Zagreb index [9], and general Randić index R_{-1} [2,12].

The line graph $L(G)$ of a graph G, $L(G) = (V_L, E_L)$, $V_L = E = \{e_1, e_2, \dots, e_m\}$, is the graph with vertex set E where two vertices e_i and e_j in $L(G)$ are adjacent, denoted as $e_i \sim e_j$, if and only if edges e_i and e_j are adjacent in G. If the end vertices of an edge $e_k \in E$, $(e_k \in V_L)$, are v_i and v_j, then the degree of e_k is defined to be $d(e_k) = d_i + d_j - 2$. The number of vertices in a line graph $L(G)$ is equal to the number of edges in G, i.e. $n_L = m$, and number of edges (see, for example, [5]) is

$$m_L = \frac{1}{2} \sum_{i\sim j} (d_i + d_j - 2).$$

The Zagreb indices of $L(G)$, that is the reformulated Zagreb indices of G, are defined as

$$\begin{aligned} EM_1(G) &= M_1(L(G)) = \sum_{i=1}^{m} d(e_i)^2 = \sum_{e_i\sim e_j} (d(e_i) + d(e_j)), \\ EM_2(G) &= M_2(L(G)) = \sum_{e_i\sim e_j} d(e_i) d(e_j), \\ EM_2^*(G) &= M_2^*(L(G)) = \sum_{e_i\sim e_j} \frac{1}{d(e_i) d(e_j)} . \end{aligned}$$

In this paper we determine the bounds of $M_2^*(G)$ on a line graph $L(G)$.

2 Main result

In the next theorem we determine a lower bound on $EM_2^*(G)$ when the size and minimum or maximum degree of the considered line graph are known.

Theorem 2.1. *Let G be a connected graph with $m \geq 2$ edges. Then we have*

$$EM_2^*(G) \geq \frac{m\delta_e - m_L}{\delta_e^2}, \tag{2.1}$$

and

$$EM_2^*(G) \geq \frac{m\Delta_e - m_L}{\Delta_e^2}. \tag{2.2}$$

Equality in (2.1) *holds if and only if in every pair of adjacent edges e_i and e_j in G, at least one has degree δ_e. Equality in* (2.2) *holds if and only if in every adjacent pairs of edges e_i and e_j in G, at least one has degree Δ_e.*

Proof. For every i and j, with $1 \leq i \leq m$ and $1 \leq j \leq m$, it holds that

$$(d(e_i) - \delta_e)(d(e_j) - \delta_e) \geq 0 \quad \text{and} \quad (\Delta_e - d(e_i))(\Delta_e - d(e_j)) \geq 0,$$

that is

$$d(e_i)d(e_j) + \delta_e^2 \geq \delta_e(d(e_i) + d(e_j)) \text{ and } d(e_i)d(e_j) + \Delta_e^2 \geq \Delta_e(d(e_i) + d(e_j)). \tag{2.3}$$

After dividing the above inequalities by $d(e_i)d(e_j)$, we obtain

$$\begin{aligned} &1 + \frac{\delta_e^2}{d(e_i)d(e_j)} \geq \delta_e\left(\frac{1}{d(e_i)} + \frac{1}{d(e_j)}\right) \quad \text{and} \\ &1 + \frac{\Delta_e^2}{d(e_i)d(e_j)} \geq \Delta_e\left(\frac{1}{d(e_i)} + \frac{1}{d(e_j)}\right). \end{aligned} \tag{2.4}$$

Now, after summing (2.4) over all pairs of adjacent edges e_i and e_j in G, we obtain

$$\sum_{e_i \sim e_j} 1 + \delta_e^2 \sum_{e_i \sim e_j} \frac{1}{d(e_i)d(e_j)} \geq \delta_e \sum_{e_i \sim e_j} \left(\frac{1}{d(e_i)} + \frac{1}{d(e_j)}\right) = \delta_e \sum_{i=1}^m 1,$$

and

$$\sum_{e_i \sim e_j} 1 + \Delta_e^2 \sum_{e_i \sim e_j} \frac{1}{d(e_i)d(e_j)} \geq \Delta_e \sum_{e_i \sim e_j} \left(\frac{1}{d(e_i)} + \frac{1}{d(e_j)}\right) = \Delta_e \sum_{i=1}^m 1,$$

that is

$$m_L + \delta_e^2 EM_2^*(G) \geq m\delta_e \quad \text{and} \quad m_L + \Delta_e^2 EM_2^*(G) \geq m\Delta_e, \tag{2.5}$$

from which we arrive at (2.1) and (2.2).

Equality in the first inequality in (2.5), and therefore in (2.1), holds if and only if in every pair of adjacent edges e_i and e_j in G, at least one is of degree δ_e. Likewise, equality in the second inequality in (2.5), and consequently in (2.2), holds if and only if in every pair of adjacent edges e_i and e_j in G, at least one is of degree Δ_e. □

Before providing some corollaries of Theorem 2.1, we prove two auxiliary results.

Lemma 2.1. *Let G be a connected graph with $m \geq 3$ edges such that $L(G)$ is non–regular, that is $\Delta_e \neq \delta_e$. If for every pair of adjacent edges e_i and e_j of G holds that $d(e_i) = \Delta_e$ and $d(e_j) = \delta_e$, or vice versa, then $G \cong P_4$.*

Proof. Contrarily, assume that there exists an edge e_i of G such that $d(e_i) = \Delta_e \geq 3$. Then, there are at least two edges e_j and e_k of G that are adjacent to e_i and also they are mutually adjacent, that is $e_j \sim e_k$. This is a contradiction to the assumption of lemma that no two adjacent edges have the same degree. This means that the assumption $d(e_i) = \Delta_e \geq 3$ was wrong and thus we must have $d(e_i) = \Delta_e \leq 2$. This implies that if two edges e_i and e_j are adjacent in G, then $d(e_i) = 2$ and $d(e_j) = 1$. Since G is connected, this is valid if and only if $m = 3$, that is $G \cong P_4$. □

Lemma 2.2. *Let G be a connected graph with $m \geq 2$ edges. Then*

$$m\delta_e \leq 2m_L \leq m\Delta_e \,. \tag{2.6}$$

Equality holds if and only if $L(G)$ is a regular graph.

Proof. Since

$$2m_L = M_1(G) - 2m = \sum_{i\sim j}(d_i + d_j - 2) = \sum_{i=1}^{m} d(e_i)\,,$$

the required result immediately follows. □

By using Lemmas 2.1 and 2.2 it is easy to prove the following corollaries of Theorem 2.1.

Corollary 2.1. *Let G be a connected graph with $m \geq 2$ edges. Then, we have*

$$EM_2^*(G) \geq \frac{m(\Delta_e + \delta_e) - 2m_L}{\Delta_e^2 + \delta_e^2}\,.$$

Equality holds if and only if either $L(G)$ is regular or $L(G) \cong P_3$.

Corollary 2.2. *Let G be a connected graph with $m \geq 2$ edges. Then, we have*

$$EM_2^*(G) \geq \frac{m}{2\Delta_e}\,.$$

Equality holds if and only if $L(G)$ is regular.

Remark 2.1. *In* [1] *it was proven that*

$$M_2^*(G) \geq \max\left\{\frac{n\delta - m}{\delta^2}, \frac{n\Delta - m}{\Delta^2}\right\}.$$

The inequalities (2.1) *and* (2.2) *are counterparts of the above inequality on a line graph $L(G)$.*

Theorem 2.2. *Let G be a connected graph with $m \geq 2$ edges. Then, we have*

$$EM_2(G) + m_L\delta_e^2 \geq \delta_e EM_1(G) \quad \text{and} \quad EM_2(G) + m_L\Delta_e^2 \geq \Delta_e EM_1(G)\,. \tag{2.7}$$

Equality in the first inequality in (2.7) *holds if and only if in every pair of adjacent edges e_i and e_j in G at least one has degree δ_e. Likewise, equality in the second inequality in* (2.7) *holds if and only if in every pair of adjacent edges e_i and e_j in G at least one has degree Δ_e.*

Proof. The required result is obtained after summation of (2.3) over all pairs of adjacent edges e_i and e_j in G. □

Remark 2.2. *In [4] the following inequalities were proven:*

$$M_2(G) + m\delta^2 \geq \delta M_1(G) \quad \text{and} \quad M_2(G) + m\Delta^2 \geq \Delta M_1(G)\,.$$

The inequalities (2.7) *are counterparts of the above inequalities on a line graph $L(G)$.*

In the next theorem we determine an upper bound on $EM_2^*(G)$ when the size and minimum and maximum degrees of the considered line graph are known.

Theorem 2.3. *Let G be a connected graph with $m \geq 2$ edges. Then, we have*

$$EM_2^*(G) \leq \frac{m(\Delta_e + \delta_e) - 2m_L}{2\Delta_e \delta_e}. \tag{2.8}$$

Equality holds if and only if $L(G)$ is regular.

Proof. For every i and j, with $1 \leq i \leq m$ and $1 \leq j \leq m$, it holds that

$$(d(e_i) - \delta_e)(\Delta_e - d(e_j)) \geq 0 \quad \text{and} \quad (\Delta_e - d(e_i))(d(e_j) - \delta_e) \geq 0,$$

that is

$$\begin{aligned} d(e_i)d(e_j) + \Delta_e\delta_e &\leq \Delta_e d(e_i) + \delta_e d(e_j), \\ d(e_i)d(e_j) + \Delta_e\delta_e &\leq \delta_e d(e_i) + \Delta_e d(e_j). \end{aligned} \tag{2.9}$$

After summing the both inequalities of (2.9) we obtain

$$2d(e_i)d(e_j) + 2\Delta_e\delta_e \leq (\Delta_e + \delta_e)(d(e_i) + d(e_j)).$$

Now, after dividing the above inequality by $d(e_i)d(e_j)$ and summing over all pairs of adjacent edges e_i and e_j of G, we obtain

$$2m_L + 2\Delta_e\delta_e EM_2^*(G) \leq m(\Delta_e + \delta_e),$$

from which (2.8) immediately follows.

Suppose that e_i and e_j are two arbitrary adjacent edges in G. Equality in the first inequality in (2.9) holds if and only if $d(e_i) = \delta_e$ or $d(e_j) = \Delta_e$. Equality in the second inequality in (2.9) holds if and only if $d(e_i) = \Delta_e$ or $d(e_j) = \delta_e$. Simultaneously, in both cases, equality holds if and only if $d(e_i) = d(e_j) = \Delta_e = \delta_e$, that is if and only if $L(G)$ is a regular graph. The equality in (2.8) holds under the same conditions. □

Corollary 2.3. *Let G be a connected graph with $m \geq 2$ edges. Then, we have*

$$EM_2^*(G) \leq \frac{m}{2\delta_e}.$$

Equality holds if and only if $L(G)$ is a regular graph.

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